Universal bounds on the electrical and elastic response of two-phase bodies and their application to bounding the volume fraction from boundary measurements

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Abstract

Universal bounds on the electrical and elastic response of two-phase (and multiphase) ellipsoidal or parallelopipedic bodies have been obtained by Nemat-Nasser and Hori. Here we show how their bounds can be improved and extended to bodies of arbitrary shape. Although our analysis is for two-phase bodies with isotropic phases it can easily be extended to multiphase bodies with anisotropic constituents. Our two-phase bounds can be used in an inverse fashion to bound the volume fractions occupied by the phases, and for electrical conductivity reduce to those of Capdeboscq and Vogelius when the volume fraction is asymptotically small. Other volume fraction bounds derived here utilize information obtained from thermal, magnetic, dielectric or elastic responses. One bound on the volume fraction can be obtained by simply immersing the body in a water filled cylinder with a piston at one end and measuring the change in water pressure when the piston is displaced by a known small amount. This bound may be particularly effective for estimating the volume of cavities in a body. We also obtain new bounds utilizing just one pair of (voltage, flux) electrical measurements at the boundary of the body.

Keywords: size estimation, universal bounds, volume fraction bounds.

1 Introduction

Berryman and Kohn (1990) found that classical variational principles could be used to obtain information about the conductivity inside a body from electrical measurements on the exterior. In this paper our main focus is on using classical variational principles and known bounds on the response of periodic composites to bound the volume fraction of one phase in a two-phase body Ω from measurements on the exterior of the body. Of course if one knows the mass densities of the two phases, the easiest way to do this is just to weigh the body. However this may not always be practical, or the densities of the two phases may be very close.

Two types of boundary conditions are most natural: what we call special Dirichlet conditions where affine Dirichlet conditions are imposed on the boundary of Ω (which

would render the field inside Ω uniform if the body were homogeneous) or what we call special Neumann conditions where Neumann conditions are imposed that would render the field inside Ω uniform if the body were homogeneous. Bounds on the electrical and elastic response of the body to these special boundary conditions were obtained by Nemat-Nasser and Hori (1993, 1995), and were extended to piezoelectricity by Hori and Nemat-Nasser (1998). They called these bounds universal because they did not depend on any assumption about the microgeometry in the body. They obtained both elementary universal bounds based on the classical variational principles, and reviewed below in section 3, and universal bounds based on the Hashin-Shtrikman variational principles (Hashin and Shtrikman 1962, 1963). The latter bounds were obtained under the assumption that Ω is either an ellipsoid or a parallelopiped, but we will see here that they can easily be improved and generalized to bodies Ω of arbitrary shape. The key is to consider an assemblage of copies of Ω packed to fill all space, and then to use the bounds of Huet (1990) which relate the effective tensor of this composite to the responses of Ω under the special boundary conditions. Then existing bounds on the effective tensor [as surveyed in the books of Nemat-Nasser and Hori (1993), Cherkaev (2000), Allaire (2002), Milton (2002), and Tartar (2009)] can be directly applied to bound the responses of Ω under special boundary conditions (see sections 5,6,7, and 8). Since these bounds involve the volume fractions of the phases (and the moduli of the phases), they can be used in an inverse fashion to bound the volume fraction. As shown by Kang, Kim, and Milton (2011) the volume fraction bounds thus obtained for electrical conductivity generalize those obtained by Capdeboscq and Vogelius (2003, 2004) for the important case when the volume fraction is asymptotically small.

Given the close connection between bounds on effective tensors and bounds on the responses of Ω under special boundary condition, a natural question to ask is whether methods that have been used to derive bounds on effective tensors could be directly used to derive bounds on the response of Ω under more general boundary conditions. One such method is the Hashin-Strikman (1962, 1963) variational method and this lead Nemat-Nasser and Hori to their bounds for ellipsoidal or parallelopipedic Ω. Another particularly successful method is the translation method (Tartar 1979; Lurie and Cherkaev 1982, 1984; Murat and Tartar 1985; Tartar 1985; Milton 1990) and indeed as shown in a companion paper (Kang, Kim, and Milton 2011) this method yields upper and lower bounds on the volume fraction in a two-phase body with general boundary conditions for two-dimensional conductivity without making any assumption on the shape of Ω. For special boundary conditions the bounds thus derived reduce to the ones derived here.

We also provide (in section 4) some new conductivity bounds which just involve the results of just one (flux, voltage) pair measured at the boundary of Ω, and which improve upon the elementary bounds of Nemat-Nasser and Hori (1993). Again these new bounds can be used in an inverse fashion to bound the volume fraction. Other volume fraction bounds using one measurement were derived by Kang, Seo, and Sheen (1997) Ikehata (1998), Alessandrini and Rosset (1998), Alessandrini, Rosset, and Seo (2000), and Alessandrini, Morassi, and Rosset (2002). These other bounds involve constants which are not easy to determine, making it difficult to make a general comparison with our new bounds.

The various bounds on the volume fraction we have derived are too numerous to summarize in this introduction. However we want to draw attention to the bounds (5.15)

and (5.24) which are the natural extension of the famous Hashin and Shtrikman (1962) conductivity bounds to this problem. Also of particular note is the bound (8.26), which is one natural generalization of the bulk modulus bounds of Hashin and Shtrikman (1963) and Hill (1963), and implies that a bound on the volume fraction can be obtained by simply immersing the body in a water filled cylinder with a piston at one end and measuring the change in water pressure when the piston is displaced by a known small amount.

2 The conductivity response tensors with special Dirichlet and special Neumann boundary conditions

In electrical impedance tomography in a body Ω containing two isotropic components with (positive, scalar) conductivities σ_1 and σ_2 the potential V satisfies

$$\nabla \cdot \sigma \nabla V = 0, \quad \text{where} \quad \sigma(\mathbf{x}) = \chi(\mathbf{x})\sigma_1 + (1 - \chi(\mathbf{x}))\sigma_2, \tag{2.1}$$

and $\chi(\mathbf{x})$ is the indicator function of component 1, taking the value 1 in component and 0 in component 2. Equivalently, in terms of the current field $\mathbf{j}(\mathbf{x})$ and electric field $\mathbf{e}(\mathbf{x})$ we have

$$\nabla \cdot \mathbf{j} = 0, \quad \mathbf{j} = \sigma\mathbf{e}, \quad \mathbf{e} = -\nabla V. \tag{2.2}$$

Let us assume the components have been labeled so that $\sigma_1 \geq \sigma_2$. We are given a set of Cauchy data, i.e. measurements of pairs (V_0, q), where $V_0(\mathbf{x})$ and $q(\mathbf{x})$ are the boundary values of the voltage $V(\mathbf{x})$ and and flux $q(\mathbf{x}) = -\mathbf{n} \cdot \mathbf{j}(\mathbf{x})$ at the boundary $\partial\Omega$ of Ω, in which $\mathbf{n}(\mathbf{x})$ is the outwards normal to the boundary. From this boundary information we can immediately determine, using integration by parts, volume averages such as

$$\langle \mathbf{e} \cdot \mathbf{j} \rangle = \frac{1}{|\Omega|} \int_{\partial\Omega} -V_0(\mathbf{j} \cdot \mathbf{n}) = \frac{1}{|\Omega|} \int_{\partial\Omega} V_0 q,$$

$$\langle \mathbf{e} \rangle = \frac{1}{|\Omega|} \int_{\partial\Omega} -V_0\mathbf{n},$$

$$\langle \mathbf{j} \rangle = \frac{1}{|\Omega|} \int_{\partial\Omega} -\mathbf{x}q, \tag{2.3}$$

where the angular brackets denote the volume average, i.e.

$$\langle g \rangle = \frac{1}{|\Omega|} \int_{\Omega} g, \tag{2.4}$$

for any quantity $g(\mathbf{x})$. From such averages our objective is to bound the volume fraction $f_1 = \langle \chi \rangle$ of component 1 (and hence also the volume fraction $f_2 = 1 - f_1$ of component 2).

To obtain good estimates of the volume fraction f_1 it makes physical sense to use measurements where the fields $\mathbf{e}(\mathbf{x})$ and $\mathbf{j}(\mathbf{x})$ probe well into the interior of Ω. In this connection two sets of measurements are most natural. We could apply special Dirichlet boundary conditions

$$V_0 = -\mathbf{e}_0 \cdot \mathbf{x}, \tag{2.5}$$

and measure $\mathbf{j}_0 = \langle \mathbf{j} \rangle$. Here, according to (2.3), $\mathbf{e}_0$ equals $\langle \mathbf{e} \rangle$. Since $\mathbf{j}_0$ is linearly related to $\mathbf{e}_0$ we can write

$$\mathbf{j}_0 = \boldsymbol{\sigma}^D \mathbf{e}_0, \tag{2.6}$$

which defines the conductivity tensor $\boldsymbol{\sigma}^D$ (D for Dirichlet). To determine $\boldsymbol{\sigma}^D$ in dimension $d = 2, 3$ it of course suffices to measure $\mathbf{j}_0$ for d linearly independent values of $\mathbf{e}_0$. Alternatively we could apply the special Neumann boundary conditions

$$q = \mathbf{j}_0 \cdot \mathbf{n}, \tag{2.7}$$

and measure $\mathbf{e}_0 = \langle \mathbf{e} \rangle$. Again according to (2.3), $\mathbf{j}_0 = \langle \mathbf{j} \rangle$. The linear relation between $\mathbf{e}_0$ and $\mathbf{j}_0$,

$$\mathbf{e}_0 = (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0 \tag{2.8}$$

defines the resistivity tensor $(\boldsymbol{\sigma}^N)^{-1}$ and hence the conductivity tensor $\boldsymbol{\sigma}^N$ (N for Neumann): we will see later that $(\boldsymbol{\sigma}^N)^{-1}$ is invertible. To determine $\boldsymbol{\sigma}^N$ it suffices to measure $\mathbf{e}_0$ for d linearly independent values of $\mathbf{j}_0$. With either of these two sorts of boundary conditions (but not in general) Hill (1963) has shown that

$$\langle \mathbf{e} \cdot \mathbf{j} \rangle = \langle \mathbf{e} \rangle \cdot \langle \mathbf{j} \rangle, \tag{2.9}$$

as follows by substituting (2.5) or (2.7) in the first of equations (2.3). Using this relationship, and its obvious generalizations, it is easy to check that both $\boldsymbol{\sigma}^D$ and $\boldsymbol{\sigma}^N$ are self-adjoint. Thus if $\mathbf{e}'(\mathbf{x})$ and $\mathbf{j}'(\mathbf{x})$ denote the electric and current fields associated with the boundary conditions (2.5), with $\mathbf{e}_0$ replaced by $\mathbf{e}_0'$, while keeping the same conductivity $\sigma(\mathbf{x})$ then

$$\mathbf{e}_0' \cdot \boldsymbol{\sigma}^D \mathbf{e}_0 = \langle \mathbf{e}' \cdot \mathbf{j} \rangle = \langle \mathbf{e}' \sigma \mathbf{e} \rangle = \langle \mathbf{e} \cdot \mathbf{j}' \rangle = \mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0', \tag{2.10}$$

which implies $\boldsymbol{\sigma}^D$ is self-adjoint. By similar argument $\boldsymbol{\sigma}^N$ is self-adjoint.

3 Known elementary bounds

This section reviews the elementary bounds on $\boldsymbol{\sigma}^D$ and $\boldsymbol{\sigma}^N$ obtained by Nemat-Nasser and Hori (1993) and by Willis in a 1989 private communication to Nemat-Nasser and Hori. Their implications for bounding the volume fraction will be studied. We will make use of two classical variational principles: the Dirichlet variational principle that

$$\min_{\substack{\underline{\mathbf{e}}(\mathbf{x}) = -\nabla \underline{V}(\mathbf{x}) \\ \underline{V}(\mathbf{x}) = V_0(\mathbf{x}) \text{ on } \partial\Omega}} \int_\Omega \underline{\mathbf{e}} \cdot \sigma \underline{\mathbf{e}} = \int_{\partial\Omega} -V_0 q, \tag{3.1}$$

which is attained when $\underline{V}(\mathbf{x}) = V(\mathbf{x})$, and the Neumann variational principle that

$$\min_{\substack{\underline{\mathbf{j}}(\mathbf{x}) \\ \nabla \cdot \underline{\mathbf{j}}(\mathbf{x}) = 0 \\ \mathbf{n} \cdot \underline{\mathbf{j}}(\mathbf{x}) = -q(\mathbf{x}) \text{ on } \partial\Omega}} \int_\Omega \underline{\mathbf{j}} \cdot \sigma^{-1} \underline{\mathbf{j}} = \int_{\partial\Omega} V_0 q, \tag{3.2}$$

4

which is attained when $\underline{j}(\mathbf{x}) = \mathbf{j}(\mathbf{x})$. With the special Dirichlet boundary conditions (2.5) the Dirichlet variational principle implies

$$\min_{\substack{\underline{\mathbf{e}}(\mathbf{x}) = -\nabla \underline{V}(\mathbf{x}) \\ \underline{V}(\mathbf{x}) = -\mathbf{e}_0 \cdot \mathbf{x} \text{ on } \partial\Omega}} \langle \underline{\mathbf{e}} \cdot \sigma \underline{\mathbf{e}} \rangle = \mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0. \tag{3.3}$$

Taking a trial potential $\underline{V} = -\mathbf{e}_0 \cdot \mathbf{x}$ produces the elementary upper bound on $\mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0$

$$\mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0 \leq \langle \sigma \rangle \mathbf{e}_0 \cdot \mathbf{e}_0, \tag{3.4}$$

given by Nemat-Nasser and Hori (1993). To obtain a lower bound observe, following a standard argument, that the left hand side of (3.3) is surely decreased if we take the minimum over a larger class of trial fields. Since the constraints on $\underline{\mathbf{e}}(\mathbf{x})$ imply $\langle \underline{\mathbf{e}} \rangle = \mathbf{e}_0$ let us replace them by this weaker constraint to obtain the inequality

$$\mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0 \geq \min_{\substack{\underline{\mathbf{e}}(\mathbf{x}) \\ \langle \underline{\mathbf{e}} \rangle = \mathbf{e}_0}} \langle \underline{\mathbf{e}} \cdot \sigma \underline{\mathbf{e}} \rangle, \tag{3.5}$$

where the minimum is now over fields $\underline{\mathbf{e}}$ which are not necessarily curl-free. Using Lagrange multipliers one finds that the minimum is attained when $\underline{\mathbf{e}} = \sigma^{-1} \langle \sigma^{-1} \rangle^{-1} \mathbf{e}_0$ and so we obtain the lower bound

$$\mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0 \geq \langle \sigma^{-1} \rangle^{-1} \mathbf{e}_0 \cdot \mathbf{e}_0 \tag{3.6}$$

of Nemat-Nasser and Hori (1993). Taken together, (3.4) and (3.6) imply the lower and upper bounds

$$\left(\frac{\mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0}{\mathbf{e}_0 \cdot \mathbf{e}_0} - \sigma_2 \right) / (\sigma_1 - \sigma_2) \leq f_1 \leq \left(\sigma_2^{-1} - \frac{\mathbf{e}_0 \cdot \mathbf{e}_0}{\mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0} \right) / (\sigma_2^{-1} - \sigma_1^{-1}) \tag{3.7}$$

on the volume fraction f_1. These bounds give useful information even if we only know $\mathbf{j}_0 = \boldsymbol{\sigma}^D \mathbf{e}_0$ for only one value of $\mathbf{e}_0$, i.e. if we only take one measurement. These bounds (3.7) are sharp in the sense that the lower bound is approached artitrarily closely if Ω is filled with a periodic laminate of components 1 and 2, oriented with the normal to the layers orthogonal to $\mathbf{e}_0$ and we let the period length go to zero, while the upper bound is approached artitrarily closely for the same geometry, but oriented with the normal to the layers parallel to $\mathbf{e}_0$. If the full tensor $\boldsymbol{\sigma}^D$ is known, from $d = 2, 3$ measurements of pairs $(\mathbf{e}_0, \mathbf{j}_0)$ then we can take the intersection of the bounds (3.7) as $\mathbf{e}_0$ is varied, and so obtain

$$(\lambda_+^D - \sigma_2)/(\sigma_1 - \sigma_2) \leq f_1 \leq (1/\sigma_2 - 1/\lambda_-^D)/(\sigma_2^{-1} - \sigma_1^{-1}), \tag{3.8}$$

where λ_+^D and λ_-^D are the maximum and minimum eigenvalues of $\boldsymbol{\sigma}^D$. However we will see in the next section that an additional and typically sharper upper bound on f_1 can be obtained.

With the special Neumann boundary conditions (2.7) the variational principle (3.2) implies

$$\min_{\substack{\underline{\mathbf{j}}(\mathbf{x}) \\ \nabla \cdot \underline{\mathbf{j}}(\mathbf{x}) = 0 \\ \mathbf{n} \cdot \underline{\mathbf{j}}(\mathbf{x}) = \mathbf{n} \cdot \mathbf{j}_0 \text{ on } \partial\Omega}} \langle \underline{\mathbf{j}} \cdot \sigma^{-1} \underline{\mathbf{j}} \rangle = \mathbf{j}_0 \cdot (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0. \tag{3.9}$$

5

By taking a constant trial field $\mathbf{j}(\mathbf{x}) = \mathbf{j}_0$ or alternatively by taking the minimum over the larger class of trial fields satisfying only $\langle \mathbf{j} \rangle = \mathbf{j}_0$ we obtain the bounds

$$\langle \sigma \rangle^{-1} \mathbf{j}_0 \cdot \mathbf{j}_0 \leq \mathbf{j}_0 \cdot (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0 \leq \langle \sigma^{-1} \rangle \mathbf{j}_0 \cdot \mathbf{j}_0 \tag{3.10}$$

of Nemat-Nasser and Hori (1993) which imply

$$\left(\frac{\mathbf{j}_0 \cdot \mathbf{j}_0}{\mathbf{j}_0 \cdot (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0} - \sigma_2 \right) / (\sigma_1 - \sigma_2) \leq f_1 \leq \left(\sigma_2^{-1} - \frac{\mathbf{j}_0 \cdot (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0}{\mathbf{j}_0 \cdot \mathbf{j}_0} \right) / (\sigma_2^{-1} - \sigma_1^{-1}). \tag{3.11}$$

These bounds are applicable even if we only know $\mathbf{e}_0 = (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0$ for only one value of $\mathbf{j}_0$. For comparison, with these special Neumann boundary conditions (2.7), the bounds in Theorem 3.1 of Kang, Seo, and Sheen (1997) coupled with the improvement in proposition 0 of Ikehata (1998), with $\sigma_1 = k > 1$, $\sigma_2 = 1$ and $\mathbf{j}_0 \cdot \mathbf{j}_0 = 1$, imply

$$\frac{1}{k-1}(1 - \mathbf{j}_0 \cdot (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0) \leq f_1 \leq \frac{k}{k-1}(1 - \mathbf{j}_0 \cdot (\boldsymbol{\sigma}^N)^{-1} \mathbf{j}_0). \tag{3.12}$$

In this case it is easy to check that the upper bounds in (3.11) and (3.12) coincide while the lower bound in (3.11) is tighter. The bounds (3.11) are each approached arbitrarily closely if Ω is filled with a periodic laminate of components 1 and 2, oriented with $\mathbf{j}_0$ either parallel or orthogonal to the layers and we let the period length go to zero.

In summary, (3.4),(3.6) and (3.10) imply the matrix inequalities

$$\langle \sigma^{-1} \rangle^{-1} \mathbf{I} \leq \boldsymbol{\sigma}^D \leq \langle \sigma \rangle \mathbf{I}, \qquad \langle \sigma^{-1} \rangle^{-1} \mathbf{I} \leq \boldsymbol{\sigma}^N \leq \langle \sigma \rangle \mathbf{I} \tag{3.13}$$

of Nemat-Nasser and Hori (1993).

For artitrary boundary conditions, i.e. for any $\mathbf{e}$ and $\mathbf{j}$ satisfying (2.2) within Ω, we have the bounds

$$\langle \mathbf{e} \cdot \mathbf{j} \rangle \geq \mathbf{e}_0 \cdot \boldsymbol{\sigma}^N \mathbf{e}_0, \quad \langle \mathbf{e} \cdot \mathbf{j} \rangle \geq \mathbf{j}_0 (\boldsymbol{\sigma}^D)^{-1} \mathbf{j}_0, \tag{3.14}$$

where $\mathbf{e}_0 = \langle \mathbf{e} \rangle$ and $\mathbf{j}_0 = \langle \mathbf{j} \rangle$, due to Willis in a 1989 private communication to Nemat-Nasser and Hori, and presented by Nemat-Nasser and Hori (1993). In conjunction with (3.13) they imply the volume fraction bounds,

$$\left(\frac{\mathbf{j}_0 \cdot \mathbf{j}_0}{\langle \mathbf{e} \cdot \mathbf{j} \rangle} - \sigma_2 \right) / (\sigma_1 - \sigma_2) \leq f_1 \leq \left(\sigma_2^{-1} - \frac{\mathbf{e}_0 \cdot \mathbf{e}_0}{\langle \mathbf{e} \cdot \mathbf{j} \rangle} \right) / (\sigma_2^{-1} - \sigma_1^{-1}). \tag{3.15}$$

4 New bounds with one measurement

If we have measurements of $\langle \mathbf{e} \cdot \mathbf{j} \rangle$ and both vectors $\mathbf{e}_0$ and $\mathbf{j}_0$ for arbitrary boundary conditions then the bounds (3.14) and (3.15) can be improved. The classical variational principle (3.1) implies

$$\min_{\substack{\underline{\mathbf{e}}(\mathbf{x}) = -\nabla \underline{V}(\mathbf{x}) \\ \underline{V}(\mathbf{x}) = V_0(\mathbf{x}) \text{ on } \partial\Omega \\ \langle \sigma \underline{\mathbf{e}} \rangle = \mathbf{j}_0}} \langle \underline{\mathbf{e}} \cdot \sigma \underline{\mathbf{e}} \rangle, = \langle \mathbf{e} \cdot \mathbf{j} \rangle \tag{4.1}$$

where we have chosen to add the constraint that $\langle \sigma \underline{\mathbf{e}} \rangle = \mathbf{j}_0$ since we know that without this constraint the minimizer $\underline{\mathbf{e}} = \mathbf{e}$ satisfies $\langle \sigma \mathbf{e} \rangle = \mathbf{j}_0$. We surely obtain something lower if take the minimum over the larger class of fields satisfying only $\langle \underline{\mathbf{e}} \rangle = \mathbf{e}_0$ and $\langle \sigma \underline{\mathbf{e}} \rangle = \mathbf{j}_0$. Thus we obtain the inequality

$$\min_{\substack{\underline{\mathbf{e}}(\mathbf{x}) \\ \langle \underline{\mathbf{e}} \rangle = \mathbf{e}_0 \\ \langle \sigma \underline{\mathbf{e}} \rangle = \mathbf{j}_0}} \langle \underline{\mathbf{e}} \cdot \sigma \underline{\mathbf{e}} \rangle \leq \langle \mathbf{e} \cdot \mathbf{j} \rangle. \tag{4.2}$$

By introducing two vector valued Lagrange multipliers associated with the two vector valued constraints we find that the minimum is attained when

$$\underline{\mathbf{e}}(\mathbf{x}) = \mathbf{e}_0 + (\langle \sigma^{-1} \rangle - \sigma^{-1}(\mathbf{x}))(\langle \sigma \rangle \langle \sigma^{-1} \rangle - 1)^{-1}(\mathbf{j}_0 - \langle \sigma \rangle \mathbf{e}_0). \tag{4.3}$$

Substituting this back in (4.2) gives the bound

$$(\langle \sigma \rangle \langle \sigma^{-1} \rangle - 1)(\langle \mathbf{e} \cdot \mathbf{j} \rangle - \mathbf{e}_0 \cdot \mathbf{j}_0) \geq (\mathbf{j}_0 - \langle \sigma \rangle \mathbf{e}_0) \cdot (\langle \sigma^{-1} \rangle \mathbf{j}_0 - \mathbf{e}_0). \tag{4.4}$$

If, with general boundary conditions, we are interested in bounding the volume fraction f_1 given measured values of $\langle \mathbf{e} \cdot \mathbf{j} \rangle$, $\mathbf{e}_0$ and $\mathbf{j}_0$ then the difference between the left hand side and right hand side of (4.4) is a quadratic in f_1 whose two roots give upper and lower bounds on f_1. (Unless the roots happen to be complex, in which case there is no configuration of the two phases within Ω which produce the measured $\langle \mathbf{e} \cdot \mathbf{j} \rangle$, $\mathbf{e}_0$ and $\mathbf{j}_0$, indicating the presence of other phases or indicating an error in measurements.)

In the particular cases of either special Dirichlet or special Neumann boundary conditions, (2.5) or (2.7), the left hand side of (4.4) vanishes (see (2.9)) and we obtain the reduced bounds

$$0 \geq (\mathbf{j}_0 - \langle \sigma \rangle \mathbf{e}_0) \cdot (\langle \sigma^{-1} \rangle \mathbf{j}_0 - \mathbf{e}_0), \tag{4.5}$$

which are in fact implied by the matrix inequalities (3.13). This bound (4.5) is optimal. For any given fixed $\mathbf{e}_0$, and fixed volume fraction f_1, the vector $\mathbf{j}_0$ has an endpoint which is constrained by (4.5) to lie within a sphere (disk in two dimensions) centered at $(\langle \sigma \rangle + \langle \sigma^{-1} \rangle^{-1}) \mathbf{e}_0/2$. When Ω is filled with a periodic laminate of the two phases with interfaces orthogonal to some unit vector $\mathbf{m}$, and we let the period length go to zero, then the endpoint of the vector $\mathbf{j}_0$ covers the entire surface of this sphere (disk) as $\mathbf{m}$ ranges over all unit vectors. These bounds are the analogs, for arbitrary bodies Ω, of bounds on possible $(\mathbf{e}_0, \mathbf{j}_0)$ pairs for composites derived by Raĭtum (1983) and Tartar (1995). If we are given $\mathbf{e}_0$ and $\mathbf{j}_0$ and want to bound f_1 then we should find the range of f_1 where the sphere (or disk) contains the endpoint of the vector $\mathbf{j}_0$. The endpoints of this range are the roots of the right hand side of (4.5) which is a quadratic function of f_1.

Knowledge of $\mathbf{e}_0$ and $\mathbf{j}_0$ is equivalent to knowledge of $\langle \mathbf{e} \cdot \mathbf{v} \rangle$ and $\langle \mathbf{v} \cdot \mathbf{j} \rangle$ for all constant fields $\mathbf{v}$. A more general alternative is to use the information about

$$a_i = \langle \mathbf{e} \cdot \mathbf{j}_i \rangle = \frac{1}{|\Omega|} \int_{\partial \Omega} -V_0 (\mathbf{j}_i \cdot \mathbf{n}),$$

$$b_k = \langle \nabla V_k \cdot \mathbf{j} \rangle = \frac{1}{|\Omega|} \int_{\partial \Omega} -V_k (\mathbf{j} \cdot \mathbf{n}), \tag{4.6}$$

7

for a given set of "comparison flux fields" $\mathbf{j}_i(\mathbf{x})$ satisfying $\nabla \cdot \mathbf{j}_i = 0$, $i = 1, 2, \ldots n$ and "comparison potentials" $V_k(\mathbf{x})$, $k = 1, 2, \ldots m$. Suppose, for example, that we have just one comparison flux field $\mathbf{j}_1$. We have the variational principle

$$\min_{\substack{\underline{\mathbf{e}}(\mathbf{x}) = -\nabla \underline{V}(\mathbf{x}) \\ \underline{V}(\mathbf{x}) = V_0(\mathbf{x}) \text{ on } \partial\Omega \\ \langle \underline{\mathbf{e}} \cdot \mathbf{j}_1 \rangle = a_1}} \langle \underline{\mathbf{e}} \cdot \sigma \underline{\mathbf{e}} \rangle = \langle \mathbf{e} \cdot \mathbf{j} \rangle, \tag{4.7}$$

where we have chosen to add the constraint that $\langle \underline{\mathbf{e}} \cdot \mathbf{j}_1 \rangle = a_1$ since we know that without this constraint the minimizer $\underline{\mathbf{e}} = \mathbf{e}$ satisfies $\langle \mathbf{e} \cdot \mathbf{j}_1 \rangle = a_1$. This implies the inequality

$$\langle \mathbf{e} \cdot \mathbf{j} \rangle \geq \min_{\substack{\underline{\mathbf{e}}(\mathbf{x}) \\ \langle \underline{\mathbf{e}} \cdot \mathbf{j}_1 \rangle = a_1}} \langle \underline{\mathbf{e}} \cdot \sigma \underline{\mathbf{e}} \rangle. \tag{4.8}$$

By introducing a Lagrange multiplier associated with the constraint $\langle \mathbf{e} \cdot \mathbf{j}_1 \rangle = a_1$ we see the minimum occurs when

$$\underline{\mathbf{e}} = a_1 \sigma^{-1} \mathbf{j}_1 / \langle \mathbf{j}_1 \cdot \sigma^{-1} \mathbf{j}_1 \rangle, \tag{4.9}$$

giving the inequality

$$\langle \mathbf{e} \cdot \mathbf{j} \rangle \geq a_1^2 / \langle \mathbf{j}_1 \cdot \sigma^{-1} \mathbf{j}_1 \rangle. \tag{4.10}$$

This inequality gives information about $\sigma(\mathbf{x})$ through $\langle \mathbf{j}_1 \cdot \sigma^{-1} \mathbf{j}_1 \rangle$. If we only want bounds which involve the volume fraction we should choose $\mathbf{j}_1(\mathbf{x})$ with

$$|\mathbf{j}_1(\mathbf{x})| = 1 \quad \text{for all } \mathbf{x} \in \Omega. \tag{4.11}$$

There are many divergence free fields $\mathbf{j}_1(\mathbf{x})$ which satisfy this constraint. For example in two dimensions we can take

$$\mathbf{j}_1 = (\partial\phi/\partial x_2, -\partial\phi/\partial x_1), \quad \text{with } |\nabla\phi(\mathbf{x})| = 1 \quad \text{for all } \mathbf{x} \in \Omega. \tag{4.12}$$

Thus $\phi(\mathbf{x})$ satisfies an Eikonal equation, and we could take $\phi(\mathbf{x})$ to be the shortest distance between $\mathbf{x}$ and a curve outside Ω. Once (4.11) is satisfied (4.10) implies the volume fraction bound

$$f_1 \leq \left(\sigma_2^{-1} - \frac{a_1^2}{\langle \mathbf{e} \cdot \mathbf{j} \rangle} \right) / (\sigma_2^{-1} - \sigma_1^{-1}). \tag{4.13}$$

In the special case when $\mathbf{j}_1 = \mathbf{e}_0/|\mathbf{e}_0|$ this reduces to the upper bound on f_1 given by (3.15).

An important question is whether this new bound is sharp, and if so for what $\sigma(\mathbf{x})$? The new bound will be sharp when $\mathbf{e} = \underline{\mathbf{e}}$ where $\underline{\mathbf{e}}$ is given by (4.9). In that case

$$\mathbf{j}(\mathbf{x}) = a_1 \mathbf{j}_1 / \langle \mathbf{j}_1 \cdot \sigma^{-1} \mathbf{j}_1 \rangle \tag{4.14}$$

has zero divergence because it is proportional to $\mathbf{j}_1$. Let us impose the Neumann boundary condition

$$\mathbf{j}(\mathbf{x}) \cdot \mathbf{n} = \mathbf{j}_1 \cdot \mathbf{n} \quad \text{for all } \mathbf{x} \in \partial\Omega, \tag{4.15}$$
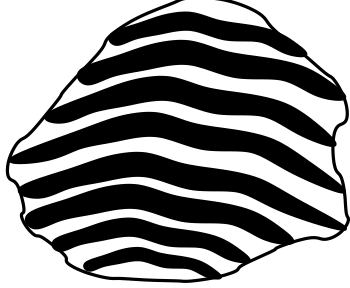
8

Figure 1: A schematic of the type of layered microstructure achieving the volume fraction bound (4.13), where the black regions denote one phase, and the white regions the other phase. The layer widths should be much finer than the size of Ω.

and look for a $\sigma(\mathbf{x})$ so $\mathbf{j}(\mathbf{x}) = \mathbf{j}_1(\mathbf{x})$ and $\mathbf{e}(\mathbf{x}) = \sigma^{-1}\mathbf{j}_1(\mathbf{x})$ is curl-free. Now as schematically represented by figure 1, choose $\sigma(\mathbf{x})$ to correspond to a finely layered composite with layers orthogonal to the streamlines of $\mathbf{j}_1(\mathbf{x})$, and with phase 1 occupying a local volume fraction $p(\mathbf{x})$. This composite will support a current field $\mathbf{j}(\mathbf{x}) = \mathbf{j}_1(\mathbf{x})$ and an electric field $\mathbf{e}(\mathbf{x}) = \sigma^{-1}\mathbf{j}_1(\mathbf{x})$ provided

$$\nabla \times \mathbf{e}_0 = 0, \quad \mathbf{e}_0 \equiv [\sigma_2^{-1} - p(\mathbf{x})(\sigma_2^{-1} - \sigma_1^{-1})]\mathbf{j}_1(\mathbf{x}). \tag{4.16}$$

Here $\mathbf{e}_0(\mathbf{x})$ is the weak limit (local volume average) of $\mathbf{e}(\mathbf{x})$ as the layer spacing goes to zero. In two dimensions, given $\mathbf{j}_1(\mathbf{x})$ we could look for solutions for $p(\mathbf{x})$ such that (4.16) is satisfied and $0 \le p(\mathbf{x}) \le 1$ in Ω. We expect such solutions to exist for a wide class of fields $\mathbf{j}_1(\mathbf{x})$. This example shows that non-constant "comparison flux fields" can lead to sharp bounds on the volume fraction. In three dimensions we only expect to find a solution of the vector equation (4.16) for the scalar field $p(\mathbf{x})$ if $\mathbf{j}_1(\mathbf{x})$ satisfies some additional conditions.

5 Relationship to bounding effective tensors of composites

Consider a periodic composite obtained by taking the unit cell boundaries outside $\Omega \equiv \Omega_1$ and almost filling the rest of the unit cell by non-intersecting rescaled and translated copies Ω_i, $i = 2, \ldots, n$ of Ω, as illustrated in figure 2. The remainder of the unit cell is filled by phase 2 with conductivity σ_2. The unit cell structure is periodically repeated to fill all space. Let $\sigma_C(\mathbf{x})$ (C for composite) denote this effective conductivity, i.e. in the
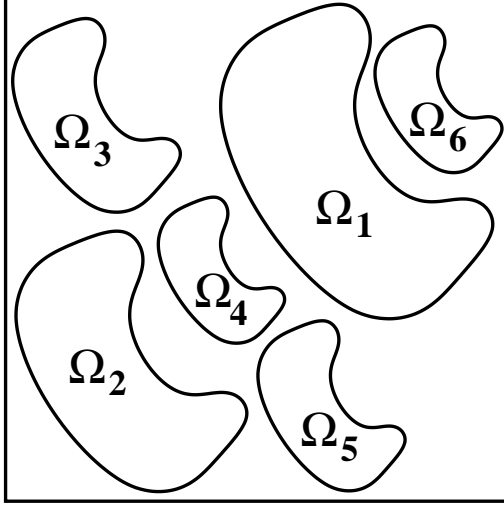
Figure 2: A period cell containing rescaled copies of Ω.

unit cell

$$\sigma_C(\mathbf{x}) = \sigma(\mathbf{x}/a_i + \mathbf{b}_i) \text{ in } \Omega_i, \quad i = 1, 2, \ldots, N$$
$$= \sigma_2 \text{ elsewhere outside } \cup_i \Omega_i, \tag{5.1}$$

where the scaling constants a_i and translation vectors $\mathbf{b}_i$ (with $a_1 = 1$ and $\mathbf{b}_1 = 0$) are determined by the size and position of each copy Ω_i, so that $\mathbf{x}/a_i + \mathbf{b}_i$ is on the boundary of Ω if and only if $\mathbf{x}$ is on the boundary of Ω_i. Let p_n denote the volume fraction in the unit cell occupied by the material with conductivity σ_2. Let $\boldsymbol{\sigma}_n^*$ denote the (matrix valued) effective conductivity of this composite, which in general depends upon the relative positions of the copies Ω_i within the unit cell.

We have the classical variational inequality

$$\mathbf{e}_0 \cdot \boldsymbol{\sigma}_n^* \mathbf{e}_0 \leq \langle \underline{\mathbf{e}}_C \cdot \sigma_C \underline{\mathbf{e}}_C \rangle, \tag{5.2}$$

which holds for any trial electric field $\underline{\mathbf{e}}_C$ satisfying

$$\nabla \times \underline{\mathbf{e}}_C = 0, \quad \underline{\mathbf{e}}_C \text{ periodic}, \quad \langle \underline{\mathbf{e}}_C \rangle = \mathbf{e}_0, \tag{5.3}$$

where now the volume averages are over the entire unit cell, rather than just Ω. In particular, letting $\mathbf{e}(\mathbf{x})$ denote the electric field within Ω when the special Dirichlet boundary conditions (2.5) are applied, we may take in the unit cell

$$\underline{\mathbf{e}}_C(\mathbf{x}) = \mathbf{e}(\mathbf{x}/a_i + \mathbf{b}_i) \text{ in } \Omega_i, \quad i = 1, 2, \ldots, N$$
$$= \mathbf{e}_0 \text{ elsewhere outside } \cup_i \Omega_i, \tag{5.4}$$

and periodically extend it. Then we get

$$\langle \underline{\mathbf{e}}_C \cdot \sigma_C \underline{\mathbf{e}}_C \rangle = p_n \sigma_2 \mathbf{e}_0 \cdot \mathbf{e}_0$$

10

$$+(1 - p_n) \sum_{i=1}^{N} \langle \mathbf{e}(\mathbf{x}/a_i + \mathbf{b}_i) \cdot \sigma(\mathbf{x}/a_i + \mathbf{b}_i) \mathbf{e}(\mathbf{x}/a_i + \mathbf{b}_i) \rangle_{\Omega_i}$$

$$= p_n \sigma_2 \mathbf{e}_0 \cdot \mathbf{e}_0 + (1 - p_n) \langle \mathbf{e}(\mathbf{x}) \cdot \sigma(\mathbf{x}) \mathbf{e}(\mathbf{x}) \rangle_{\Omega}$$

$$= p_n \sigma_2 \mathbf{e}_0 \cdot \mathbf{e}_0 + (1 - p_n) \mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0, \tag{5.5}$$

where $\langle \cdot \rangle_{\Omega_i}$ denotes an average over the region Ω_i. Combined with the variational inequality (5.2) this implies the bound

$$\mathbf{e}_0 \cdot \boldsymbol{\sigma}_n^* \mathbf{e}_0 \leq p_n \sigma_2 \mathbf{e}_0 \cdot \mathbf{e}_0 + (1 - p_n) \mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0 \leq \mathbf{e}_0 \cdot \boldsymbol{\sigma}^D \mathbf{e}_0, \tag{5.6}$$

where we have used the inequality $\boldsymbol{\sigma}^D \geq \sigma_2 \mathbf{I}$ implied by (3.13). Thus we get

$$\boldsymbol{\sigma}_n^* \leq \boldsymbol{\sigma}^D. \tag{5.7}$$

This composite has a volume fraction $f_1' = (1 - p_n) f_1$ of phase 1. Thus any bound "from below" on the effective conductivity $\boldsymbol{\sigma}_n^*$, applicable to composites having a volume fraction f_1' of phase 1, immediately translates into bound "from below" on $\boldsymbol{\sigma}^D$. Now consider what happens as we increase N, inserting more and more regions Ω_i, while leaving undisturbed the regions Ω_i already in place, so that $p_n \to 0$ as $n \to \infty$. We are assured that this is possible. Rescaled copies of any shaped region can be packed to fill all space: see, for example, Theorem A.1 in Benveniste and Milton (2003). Define

$$\boldsymbol{\sigma}^* = \lim_{n \to \infty} \boldsymbol{\sigma}_n^*. \tag{5.8}$$

We are assured this limit exists since if we change the geometry in some small volume then the effective conductivity (assuming σ_1 and σ_2 are strictly positive and finite) is perturbed only by a small amount (Zhikov, Kozlov, and Oleinik 1994). We will call $\boldsymbol{\sigma}^*$ the effective conductivity tensor of an assemblage of rescaled copies of Ω packed to fill all space. Then (5.7) implies

$$\boldsymbol{\sigma}^* \leq \boldsymbol{\sigma}^D, \tag{5.9}$$

which is essentially the bound of Huet (1990) applied to this assemblage. Assume the bound is continuous with respect to f_1' at the point $f_1' = f_1$, as expected. Then taking the limit $n \to \infty$ the "lower bound" on the effective tensor of composites having volume fraction f_1 must also be a lower bound on $\boldsymbol{\sigma}^D$.

In particular, the harmonic mean bound $\boldsymbol{\sigma}^* \geq \langle \sigma^{-1} \rangle^{-1} \mathbf{I}$ translates into the elementary bound $\boldsymbol{\sigma}^D \geq \langle \sigma^{-1} \rangle^{-1} \mathbf{I}$ of Nemat-Nasser and Hori, obtained before. Additionally, in our two-phase composite, the effective conductivity $\boldsymbol{\sigma}^*$ satisfies the Lurie-Cherkaev-Murat-Tartar bound (Lurie and Cherkaev 1982, 1984; Murat and Tartar 1985; Tartar 1985)

$$f_1 \mathrm{Tr}[(\boldsymbol{\sigma}^* - \sigma_2 \mathbf{I})^{-1}] \leq d/(\sigma_1 - \sigma_2) + f_2/\sigma_2, \tag{5.10}$$

[which are a generalization of the bounds of Hashin and Shtrikman (1962)] where $d = 2, 3$ is the dimensionality of the composite. Since $\boldsymbol{\sigma}^D \geq \boldsymbol{\sigma}^* \geq \sigma_2 \mathbf{I}$ it follows that

$$(\boldsymbol{\sigma}^* - \sigma_2 \mathbf{I})^{-1} \geq (\boldsymbol{\sigma}^D - \sigma_2 \mathbf{I})^{-1}, \tag{5.11}$$

and so (5.10) implies the new bound

$$f_1 \mathrm{Tr}[(\boldsymbol{\sigma}^D - \sigma_2 \mathbf{I})^{-1}] \leq d/(\sigma_1 - \sigma_2) + f_2/\sigma_2. \tag{5.12}$$

11

By multiplying this inequality by σ_2^2 and adding $df_1\sigma_2$ to both sides we see that it can be rewritten in the equivalent form

$$f_1 \text{Tr}[(\sigma_2^{-1}\mathbf{I} - (\boldsymbol{\sigma}^D)^{-1})^{-1}] \leq d/(\sigma_2^{-1} - \sigma_1^{-1}) - (d-1)f_2\sigma_2. \tag{5.13}$$

As $d^2/\text{Tr}(\mathbf{A}) \leq \text{Tr}(\mathbf{A}^{-1})$ for any positive definite matrix $\mathbf{A}$ we also obtain the weaker bound

$$\frac{1}{d}\text{Tr}[(\boldsymbol{\sigma}^D)^{-1}] \leq \sigma_2^{-1} - \frac{f_1 d}{d/(\sigma_2^{-1} - \sigma_1^{-1}) - (d-1)f_2\sigma_2}, \tag{5.14}$$

which is a particular case of the universal bounds first derived by Nemat-Nasser and Hori (1993, 1995), see equation (5.4.9) in their 1995 paper, obtained under the assumption that Ω is ellipsoidal or parallelpipedic. (which we see is not needed).

If one is interested in bounds on the volume fraction f_1 then (5.12) implies the upper bound

$$f_1 \leq \frac{1/\sigma_2 + d/(\sigma_1 - \sigma_2)}{1/\sigma_2 + \text{Tr}[(\boldsymbol{\sigma}^D - \sigma_2\mathbf{I})^{-1}]}. \tag{5.15}$$

To obtain lower bounds on f_1, we consider the same periodic composite and apply the dual variational inequality

$$\mathbf{j}_0 \cdot (\boldsymbol{\sigma}_n^*)^{-1}\mathbf{j}_0 \leq \langle \underline{\mathbf{j}}_C \cdot \sigma_C^{-1}\underline{\mathbf{j}}_C \rangle \tag{5.16}$$

valid for any trial current field $\underline{\mathbf{j}}_C$ satisfying

$$\nabla \cdot \underline{\mathbf{j}}_C = 0, \quad \underline{\mathbf{j}}_C \text{ periodic}, \quad \langle \underline{\mathbf{j}}_C \rangle = \mathbf{j}_0. \tag{5.17}$$

Letting $\mathbf{j}(\mathbf{x})$ denote the current field within Ω when the special Neumann boundary conditions (2.7) are applied, we may take in the unit cell

$$\begin{aligned}
\underline{\mathbf{j}}_C(\mathbf{x}) &= \mathbf{j}(\mathbf{x}/a_i + \mathbf{b}_i) \text{ in } \Omega_i, \quad i = 1, 2, \ldots, N \\
&= \mathbf{j}_0 \text{ elsewhere outside } \cup_i \Omega_i,
\end{aligned} \tag{5.18}$$

and periodically extend it. Substituting this trial field in (5.16) gives the bound

$$(\boldsymbol{\sigma}_n^*)^{-1} \leq p_n\sigma_2^{-1}\mathbf{I} + (\boldsymbol{\sigma}^N)^{-1}, \tag{5.19}$$

which in the limit $n \to \infty$ implies

$$\boldsymbol{\sigma}^* \geq \boldsymbol{\sigma}^N, \tag{5.20}$$

which is essentially the bound of Huet (1990) applied to the assemblage of rescaled copies of Ω packed to fill all space.

Thus any bound "from above" on the effective conductivity $\boldsymbol{\sigma}_n^*$ of composites having a volume fraction f_1' immediately translates into a bound "from above" on $(p_n\sigma_2^{-1}\mathbf{I} + (\boldsymbol{\sigma}^N)^{-1})^{-1}$. Taking the limit $n \to \infty$ and assuming continuity of the bound at $f_1' = f_1$ the "upper bound" on the effective tensor of composites having volume fraction f_1 must also be an upper bound on $\boldsymbol{\sigma}^N$. In particular, the other Murat-Tartar-Lurie-Cherkaev bound

$$f_2\text{Tr}[(\sigma_1\mathbf{I} - \boldsymbol{\sigma}^*)^{-1}] \leq d/(\sigma_1 - \sigma_2) - f_1/\sigma_1, \tag{5.21}$$

implies

$$f_2\text{Tr}[(\sigma_1\mathbf{I} - \boldsymbol{\sigma}^N)^{-1}] \leq d/(\sigma_1 - \sigma_2) - f_1/\sigma_1. \tag{5.22}$$

12

Again using the inequality $d^2/\text{Tr}(\mathbf{A}) \leq \text{Tr}(\mathbf{A}^{-1})$ for $\mathbf{A} > 0$, we obtain the weaker bound

$$\frac{1}{d}\text{Tr}(\boldsymbol{\sigma}^N) \leq \sigma_1 - \frac{f_2 d}{d/(\sigma_1 - \sigma_2) - f_1/\sigma_1} \tag{5.23}$$

which is a particular case of the universal bounds derived by Nemat-Nasser and Hori (1993, 1995), see equation (5.3.11) in their 1995 paper, obtained under the assumption that Ω is ellipsoidal or parallelpipedic (which we see is not needed).

From (5.22) we directly obtain the volume fraction bound

$$f_2 \leq \frac{d/(\sigma_1 - \sigma_2) - 1/\sigma_1}{\{\text{Tr}[(\sigma_1\mathbf{I} - \boldsymbol{\sigma}^N)^{-1}]\} - 1/\sigma_1}, \tag{5.24}$$

giving a lower bound on the volume fraction $f_1 = 1 - f_2$.

In the asymptotic limit as the volume fraction goes to zero the volume fraction bounds (5.15) and (5.24) reduce to those of Capdeboscq and Vogelius (2003, 2004), as shown in the two dimensional case by Kang, Kim, and Milton (2011). The paper of Kang, Kim and Milton also tests the bounds numerically, and their (two-dimensional) results show the bound (5.15) is typically close to the actual volume fraction for a variety of inclusions of phase 1 in a matrix of phase 2. Similarly we can expect that the bound (5.24) will be typically close to the actual volume fraction for a variety of inclusions of phase 2 in a matrix of phase 1.

6   Coupled bounds in two-dimensions

The tensors $\boldsymbol{\sigma}^D$ and $\boldsymbol{\sigma}^N$ obviously depend on σ_1 and σ_2, i.e. $\boldsymbol{\sigma}^D = \boldsymbol{\sigma}^D(\sigma_1, \sigma_2)$ and $\boldsymbol{\sigma}^N = \boldsymbol{\sigma}^N(\sigma_1, \sigma_2)$. Let us assume we have measurements of these tensors for an additional pair of conductivities (k_1, k_2), (which could be obtained, say from thermal, magnetic permeability, or diffusivity measurements) and let $\mathbf{k}^D$ and $\mathbf{k}^N$ denote these tensors,

$$\mathbf{k}^D = \boldsymbol{\sigma}^D(k_1, k_2), \quad \mathbf{k}^N = \boldsymbol{\sigma}^N(k_1, k_2). \tag{6.1}$$

We still let $\boldsymbol{\sigma}^D$ and $\boldsymbol{\sigma}^N$ denote the tensors associated with the first pair of conductivities (σ_1, σ_2), with $\sigma_1 > \sigma_2$. From (5.9) and (5.20) we have the inequalities

$$\sigma_2\mathbf{I} \leq \boldsymbol{\sigma}^N \leq \boldsymbol{\sigma}^* \leq \boldsymbol{\sigma}^D \leq \sigma_1\mathbf{I},$$
$$k^- \leq \mathbf{k}^N \leq \mathbf{k}^* \leq \mathbf{k}^D \leq k^+\mathbf{I}, \tag{6.2}$$

where $k^- = \min\{k_1, k_2\}$ and $k^+ = \max\{k_1, k_2\}$ and $\mathbf{k}^*$ is the effective conductivity the composite considered in the previous section when σ_1 and σ_2 are replaced by k_1 and k_2. (It can easily be checked that these inequalities still hold if $k_2 > k_1$.)

For two dimensional conductivity from duality (Keller 1964; Dykhne 1970) we know the functions $\boldsymbol{\sigma}^D = \boldsymbol{\sigma}^D(\sigma_1, \sigma_2)$ and $\boldsymbol{\sigma}^N = \boldsymbol{\sigma}^N(\sigma_1, \sigma_2)$ satisfy

$$\boldsymbol{\sigma}^D(\sigma_2, \sigma_1) = \sigma_1\sigma_2\mathbf{R}_\perp^T[\boldsymbol{\sigma}^N(\sigma_1, \sigma_2)]^{-1}\mathbf{R}_\perp,$$
$$\boldsymbol{\sigma}^N(\sigma_2, \sigma_1) = \sigma_1\sigma_2\mathbf{R}_\perp^T[\boldsymbol{\sigma}^D(\sigma_1, \sigma_2)]^{-1}\mathbf{R}_\perp, \tag{6.3}$$

where

$$\mathbf{R}_\perp = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{6.4}$$

13

is the matrix for a 90° rotation. So if we know these tensors for the conductivity pair (k_1, k_2), we also know them for the conductivity pair (k_2, k_1). Hence, by making such an interchange if necessary, we may assume without loss of generality that $k_1 > k_2$, i.e. that $k^+ = k_1$ and $k^- = k_2$. Finally, by interchanging k with σ if necessary, we may assume without loss of generality that

$$\sigma_1/\sigma_2 \geq k_1/k_2 > 1. \tag{6.5}$$

Optimal bounds on all possible matrix pairs $(\boldsymbol{\sigma}^*, \mathbf{k}^*)$ for composites having a pre-scribed volume fraction f_1 of phase 1 have been derived by Cherkaev and Gibiansky (1992), and extended to an arbitrary number of effective conductivity function values by Clark and Milton (1933). However it seems difficult to extract bounds on f_1 from these optimal bounds. Instead we consider a polycrystal checkerboard with conductivities

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{R}^T(\mathbf{x})\boldsymbol{\sigma}^*\mathbf{R}(\mathbf{x}), \quad \mathbf{k}(\mathbf{x}) = \mathbf{R}^T(\mathbf{x})\mathbf{k}^*\mathbf{R}(\mathbf{x}), \quad \text{with } \mathbf{R}^T(\mathbf{x})\mathbf{R}(\mathbf{x}) = \mathbf{I}, \tag{6.6}$$

in which the rotation field $\mathbf{R}(\mathbf{x})$ is $\mathbf{I}$ in the "white squares" and $\mathbf{R}_\perp$ in the "black squares". By a result of Dykhne (1970) this material has effective conductivities $(\sigma_*\mathbf{I}, k_*\mathbf{I})$ where

$$\sigma_* = \sqrt{\det \boldsymbol{\sigma}^*}, \quad k_* = \sqrt{\det \mathbf{k}^*}. \tag{6.7}$$

Now we replace the "white squares" by the limiting composite considered in the previous section (with structure much smaller than the size of the squares) and we replace the "black squares" by the limiting composite considered in the previous section, rotated by 90°. The resulting material is an isotropic composite of phases 1 and 2 and so the pair (σ_*, k_*) satisfies the bounds of Milton (1981b),

$$u(k_*) \leq \sigma_* \leq v(k_*), \tag{6.8}$$

which are attained when the composite is an assemblage of doubly coated disks, where

$$v(k_*) = \sigma_1 - \frac{2f_2\sigma_1(\sigma_1^2 - \sigma_2^2)}{(f_2\sigma_1 + f_1\sigma_2 + \sigma_1)(\sigma_1 + \sigma_2) + (\sigma_1 - \sigma_2)^2\alpha_1(k_*)},$$
$$u(k_*) \equiv \sigma_2 + \frac{2f_1\sigma_2(\sigma_1^2 - \sigma_2^2)}{(f_2\sigma_1 + f_1\sigma_2 + \sigma_2)(\sigma_1 + \sigma_2) + (\sigma_1 - \sigma_2)^2\alpha_2(k_*)}, \tag{6.9}$$

and

$$\alpha_1(k_*) = \frac{(k_1 + k_2)[2f_2k_1(k_1 - k_2)/(k_1 - k_*) - (f_2k_1 + f_1k_2 + k_1)]}{(k_1 - k_2)^2},$$
$$\alpha_2(k_*) = \frac{(k_1 + k_2)[2f_1k_2(k_1 - k_2)/(k_* - k_2) - (f_2k_1 + f_1k_2 + k_2)]}{(k_1 - k_2)^2}. \tag{6.10}$$

Now for any two symmetric matrices $\mathbf{A}$ and $\mathbf{B}$ with $\mathbf{A} \geq \mathbf{B} > 0$ we have $\mathbf{B}^{-1/2}\mathbf{A}\mathbf{B}^{-1/2} \geq \mathbf{I}$, and so $\det(\mathbf{B}^{-1/2}\mathbf{A}\mathbf{B}^{-1/2}) \geq 1$ implying $\det(\mathbf{A}) > \det(\mathbf{B})$. Thus (6.2) and (6.7) imply

$$\sigma_2 \leq \sigma_N \leq \sigma_* \leq \sigma_D \leq \sigma_1, \quad k_2 \leq k_N \leq k_* \leq k_D \leq k_1, \tag{6.11}$$

where we define

$$\sigma_N = \sqrt{\det \boldsymbol{\sigma}_N}, \quad \sigma_D = \sqrt{\det \boldsymbol{\sigma}_D}, \quad k_N = \sqrt{\det \mathbf{k}_N}, \quad k_D = \sqrt{\det \mathbf{k}_D}. \tag{6.12}$$

14

The Hashin-Shtrikman bounds (Hashin and Shtrikman 1962; Hashin 1970),

$$k_1 - \frac{2f_2 k_1(k_1 - k_2)}{f_2 k_1 + f_1 k_2 + k_1} \geq k_* \geq k_2 + \frac{2f_1 k_2(k_1 - k_2)}{f_2 k_1 + f_1 k_2 + k_2}, \tag{6.13}$$

imply that both $\alpha_1(k_*)$ and $\alpha_2(k_*)$ are non-negative. Hence the denominators in (6.9) are positive and so (6.8) implies

$$(\sigma_1 - \sigma_*)[(f_2\sigma_1 + f_1\sigma_2 + \sigma_1)(\sigma_1 + \sigma_2) + (\sigma_1 - \sigma_2)^2\alpha_1(k_*)] \geq 2f_2\sigma_1(\sigma_1^2 - \sigma_2^2),$$
$$(\sigma_* - \sigma_2)[(f_2\sigma_1 + f_1\sigma_2 + \sigma_2)(\sigma_1 + \sigma_2) + (\sigma_1 - \sigma_2)^2\alpha_2(k_*)] \geq 2f_1\sigma_2(\sigma_1^2 - \sigma_2^2). \tag{6.14}$$

Since $\alpha_1(k_D) \geq \alpha_1(k_*)$ and $\alpha_2(k_N) \geq \alpha_2(k_*)$, we get using (6.11),

$$(\sigma_1 - \sigma_N)[(f_2\sigma_1 + f_1\sigma_2 + \sigma_1)(\sigma_1 + \sigma_2) + (\sigma_1 - \sigma_2)^2\alpha_1(k_D)] \geq 2f_2\sigma_1(\sigma_1^2 - \sigma_2^2),$$
$$(\sigma_D - \sigma_2)[(f_2\sigma_1 + f_1\sigma_2 + \sigma_2)(\sigma_1 + \sigma_2) + (\sigma_1 - \sigma_2)^2\alpha_2(k_N)] \geq 2f_1\sigma_2(\sigma_1^2 - \sigma_2^2). \tag{6.15}$$

As $\alpha_1(k_D)$ and $\alpha_2(k_N)$ depend linearly on f_1 and $f_2 = 1 - f_1$, the equations (6.15) readily yield bounds on the volume fraction. Eunjoo Kim has used an integral equation solver [as described by Kang, Kim, and Milton (2011)] to compare the bounds (6.15) with the bounds (5.15) and (5.24). Her results are presented in figures 3, 4, and 5. More numerical results testing the bounds (5.15) and (5.24) are in the paper by Kang, Kim, and Milton (2011).
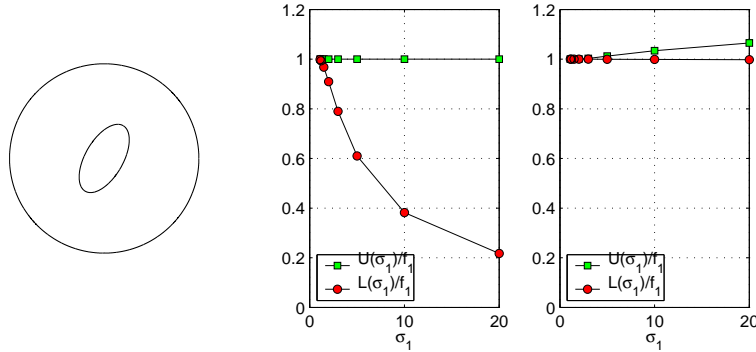

Figure 3: The first figure shows the circular body Ω containing an ellipse of phase 1 surrounded by phase 2. The second figure shows the results for the bounds (5.15) and (5.24) while the third figure shows the results for the bounds (6.15). The bounds are for increasing σ_1, with $\sigma_2 = 1$ and (for the third figure) the pairs (σ_1, k_1) are taken as $(1.1, 1.05)$, $(1.2, 1.1)$, $(1.5, 1.2)$, $(2, 1.5)$, $(3, 2)$, $(5, 3)$, $(10, 5)$ and $(20, 10)$, with $\sigma_2 = k_2 = 1$. Here $U(\sigma_1)$ and $L(\sigma_1)$ are the upper and lower bounds on the volume fraction, and the true volume fraction is $f_1 = 0.08$. Figure supplied courtesy of Eunjoo Kim.

7 Coupled bounds in three-dimensions

We can also derive coupled bounds in three dimensions. Let us assume the phases have been labeled so that

$$\sigma_1 k_1 \geq \sigma_2 k_2, \quad \text{i.e. } \sigma_1/\sigma_2 \geq k_2/k_1, \tag{7.1}$$
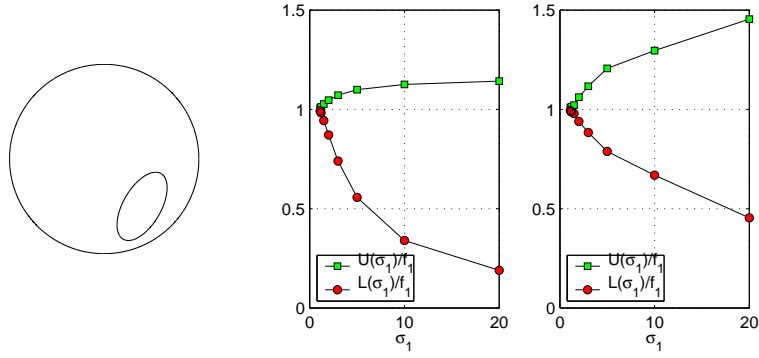
15

Figure 4: The same as for figure 3 but with the elliptical inclusion moved closer to the boundary of Ω. Figure supplied courtesy of Eunjoo Kim.
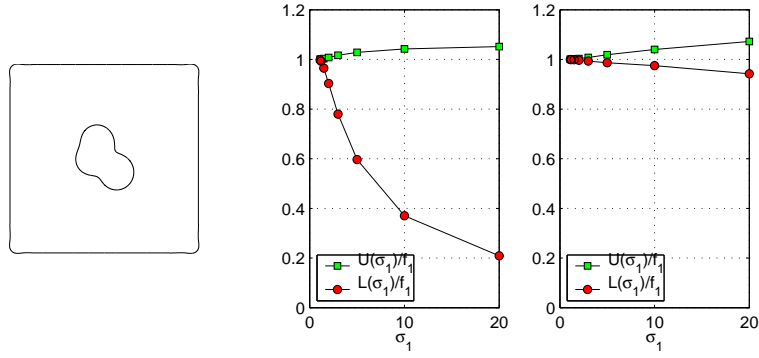

Figure 5: The same as for figure 3 but with a non-elliptical inclusion of phase 1 in a square region Ω. The true volume fraction is $f_1 = 0.0673$. Figure supplied courtesy of Eunjoo Kim.

16

and by interchanging σ with k if necessary let us assume

$$\sigma_1/\sigma_2 \geq k_1/k_2. \tag{7.2}$$

These two inequalities imply $\sigma_1/\sigma_2 > 1$ as before. We want to use the inequalities (6.2) to derive bounds on the volume fraction. As in the two-dimensional case the idea is to first construct an isotropic polycrystal, where the polycrystal has the conductivities (6.6) in which the rotation field $\mathbf{R}(\mathbf{x})$ is constant within grains which we take to be spheres. These spheres fill all space, and the crystal orientation varies randomly from sphere to sphere so that the composite has isotropic conductivities $(\sigma_*\mathbf{I}, k_*\mathbf{I})$. We use the effective medium formula (Stroud 1975; Helsing and Helte 1991) which gives

$$\sigma_* = g(\boldsymbol{\sigma}_*), \quad k_* = g(\mathbf{k}_*), \tag{7.3}$$

where for any positive definite symmetric 3×3 matrix $\mathbf{A}$, $g = g(\mathbf{A})$ is taken to be the unique positive root of

$$\frac{\lambda_1 - g}{\lambda_1 + 2g} + \frac{\lambda_2 - g}{\lambda_2 + 2g} + \frac{\lambda_3 - g}{\lambda_3 + 2g} = 0, \tag{7.4}$$

in which λ_1, λ_2, and λ_3 are the eigenvalues of $\mathbf{A}$. This effective medium formula is realizable (Milton 1985; Avellaneda 1987) in the sense that it corresponds to a limiting composite of spherical grains with hierarchical structure (where any pair of grains of comparable size are well separated from each other, relative to their diameter). Note that the left hand side of side of (7.4) increases if any of the eigenvalues λ_i increase, and decreases if g increases. So $g(\mathbf{A})$ must increase if any or all of the eigenvalues of $\mathbf{A}$ increase. It follows that $g(\mathbf{B}) \geq g(\mathbf{A})$ if $\mathbf{B} \geq \mathbf{A} > 0$. Hence the inequalities (6.2) imply

$$\sigma_2 \leq \sigma_N \leq \sigma_* \leq \sigma_D \leq \sigma_1, \quad k^- \leq k_N \leq k_* \leq k_D \leq k^+, \tag{7.5}$$

where now

$$\sigma_N = g(\boldsymbol{\sigma}_N), \quad \sigma_D = g(\boldsymbol{\sigma}_D), \quad k_N = g(\mathbf{k}_N), \quad k_D = g(\mathbf{k}_D). \tag{7.6}$$

We next replace the material in each sphere by the appropriately oriented limiting composite considered in the previous section (with structure much smaller than the sphere diameter) to obtain a two-phase isotropic composite with (σ_*, k_*) as its conductivities. Thus σ_* must satisfy the upper bound of Bergman (1976,1978)

$$\sigma_* \leq f_1\sigma_1 + f_2\sigma_2 - \frac{f_1 f_2 (\sigma_1 - \sigma_2)^2}{3\sigma_2 + (\sigma_1 - \sigma_2)\gamma(k_*)}, \tag{7.7}$$

where

$$\gamma(k_*) = \frac{f_1 f_2 (k_1 - k_2)}{f_1 k_1 + f_2 k_2 - k_*} - \frac{3k_2}{k_1 - k_2}, \tag{7.8}$$

and the lower bound

$$\sigma_* \geq \sigma_2 + \frac{3 f_1 \sigma_2 (\sigma_1 - \sigma_2)(\sigma_2 + 2\sigma_1)}{(f_2\sigma_1 + f_1\sigma_2 + 2\sigma_2)(\sigma_2 + 2\sigma_1) + (\sigma_1 - \sigma_2)^2 \beta(k_*)}, \tag{7.9}$$

17

where

$$\beta(k_*) = \frac{(k_2 + 2k_1)[3f_1k_2(k_1 - k_2)/(k_* - k_2) - (f_2k_1 + f_1k_2 + 2k_2)]}{(k_1 - k_2)^2}. \tag{7.10}$$

This lower bound was first conjectured by Milton (1981b). A proof was proposed by Avellaneda, Cherkaev, Lurie, and Milton (1988) which was corrected by Nesi (1991) and Zhikov (1991).

The lower bound (7.9) is sharp, being attained for two-phase assemblages of doubly coated spheres (Milton 1981b). The upper bound (7.7) is attained at 5 values of $\gamma(k_*)$ namely when $\gamma(k_*) = f_2, 3f_2/2, 3f_2, 3 - 3f_1/2$, and $3 - f_1$ (Milton 1981a).

The Hashin-Shtrikman bound (Hashin and Shtrikman 1962),

$$(k_* - k_2)/(k_1 - k_2) \geq 3f_1k_2/(f_2k_1 + f_1k_2 + 2k_2), \tag{7.11}$$

implies that $\beta(k_*)$ is non-negative. Hence the denominator in (7.9) is positive and so the inequality implies

$$(\sigma_* - \sigma_2)[(f_2\sigma_1 + f_1\sigma_2 + 2\sigma_2)(\sigma_2 + 2\sigma_1) + (\sigma_1 - \sigma_2)^2\beta(k_*)] \geq 3f_1\sigma_2(\sigma_1 - \sigma_2)(\sigma_2 + 2\sigma_1). \tag{7.12}$$

The Hashin-Shtrikman bounds can also be rewritten in the form

$$f_2k_1 + f_1k_2 + 2k^- \leq \frac{f_1f_2(k_1 - k_2)^2}{f_1k_1 + f_2k_2 - k_*} \leq f_2k_1 + f_1k_2 + 2k^+. \tag{7.13}$$

These inequalities imply $\gamma(k_*)$ lies between f_2 and $3 - f_1$. Hence the denominator in (7.7) is positive and the inequality can be rewritten as

$$(f_1\sigma_1 + f_2\sigma_2 - \sigma_*)(3\sigma_2 + (\sigma_1 - \sigma_2)\gamma(k_*)) \geq f_1f_2(\sigma_1 - \sigma_2)^2. \tag{7.14}$$

When $k_1 \geq k_2$ (7.5) implies $\beta(k_N) \geq \beta(k_*)$ and $\gamma(k_D) \geq \gamma(k_*)$, and hence

$$(\sigma_D - \sigma_2)[(f_2\sigma_1 + f_1\sigma_2 + 2\sigma_2)(\sigma_2 + 2\sigma_1) + (\sigma_1 - \sigma_2)^2\beta(k_N)] \geq 3f_1\sigma_2(\sigma_1 - \sigma_2)(\sigma_2 + 2\sigma_1),$$
$$(f_1\sigma_1 + f_2\sigma_2 - \sigma_N)(3\sigma_2 + (\sigma_1 - \sigma_2)\gamma(k_D)) \geq f_1f_2(\sigma_1 - \sigma_2)^2. \tag{7.15}$$

On the other hand when $k_1 \leq k_2$ then (7.5) implies $\beta(k_D) \geq \beta(k_*)$ and $\gamma(k_N) \geq \gamma(k_*)$, and hence

$$(\sigma_D - \sigma_2)[(f_2\sigma_1 + f_1\sigma_2 + 2\sigma_2)(\sigma_2 + 2\sigma_1) + (\sigma_1 - \sigma_2)^2\beta(k_D)] \geq 3f_1\sigma_2(\sigma_1 - \sigma_2)(\sigma_2 + 2\sigma_1),$$
$$(f_1\sigma_1 + f_2\sigma_2 - \sigma_N)(3\sigma_2 + (\sigma_1 - \sigma_2)\gamma(k_N)) \geq f_1f_2(\sigma_1 - \sigma_2)^2. \tag{7.16}$$

Since $\beta(k_N)$ and $\beta(k_D)$ depend linearly on the volume fractions f_1 and $f_2 = 1 - f_1$, the first inequalities in (7.15) and (7.16) also depend linearly on the volume fraction and easily yield bounds on the volume fraction. On the other hand, finding bounds on the volume fraction from the second inequalities in (7.15) and (7.16), involves solving a cubic equation in f_1. So instead of analytically computing the roots of this cubic it is probably better to numerically search for the range of values of f_1 where the second inequalities in (7.15) and (7.16) are satisfied.

8   Bounds for elasticity

Let us consider solutions to the linear elasticity equations

$$\boldsymbol{\tau}(\mathbf{x}) = \boldsymbol{\mathcal{C}}(\mathbf{x})\boldsymbol{\epsilon}(\mathbf{x}), \quad \nabla \cdot \boldsymbol{\theta} = 0, \quad \boldsymbol{\epsilon} = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2, \tag{8.1}$$

within Ω, where $\mathbf{u}(\mathbf{x})$, $\boldsymbol{\epsilon}(\mathbf{x})$ and $\boldsymbol{\tau}(\mathbf{x})$, are the displacement field, strain field, and stress field, and $\boldsymbol{\mathcal{C}}(\mathbf{x})$ is the fourth order elasticity tensor field

$$\boldsymbol{\mathcal{C}}(\mathbf{x}) = \chi(\mathbf{x})\boldsymbol{\mathcal{C}}^1 + (1 - \chi(\mathbf{x}))\boldsymbol{\mathcal{C}}^2, \tag{8.2}$$

in which $\boldsymbol{\mathcal{C}}^1$ and $\boldsymbol{\mathcal{C}}^2$ are the elasticity tensors of the phases, assumed to be isotropic with elements,

$$\mathcal{C}^h_{ijk\ell} = \mu_h(\delta_{ik}\delta_{j\ell} + \delta_{i\ell}\delta_{jk}) + (\kappa_h - 2\mu_h/d)\delta_{ij}\delta_{k\ell}, \quad h = 1, 2, \tag{8.3}$$

in which $d = 2$ or 3 is the dimensionality, and μ_1, μ_2 and κ_1, κ_2 are the shear and bulk moduli of the two phases. From boundary information on the displacement $\mathbf{u}_0(\mathbf{x}) = \mathbf{u}(\mathbf{x})$ and traction $\mathbf{f}(\mathbf{x}) = \boldsymbol{\tau}(\mathbf{x}) \cdot \mathbf{n}$ we can immediately determine, using integration by parts, volume averages such as

$$\langle \boldsymbol{\epsilon} : \boldsymbol{\tau} \rangle = \frac{1}{|\Omega|} \int_{\partial\Omega} \mathbf{u} \cdot \mathbf{f},$$

$$\langle \boldsymbol{\epsilon} \rangle = \frac{1}{|\Omega|} \int_{\partial\Omega} (\mathbf{n}\mathbf{u}^T + \mathbf{u}\mathbf{n}^T)/2,$$

$$\langle \boldsymbol{\tau} \rangle = \frac{1}{|\Omega|} \int_{\partial\Omega} \mathbf{x}\mathbf{f}^T, \tag{8.4}$$

in which " : " denotes a contraction of two indices.

There are two natural sets of boundary conditions. For any symmetric matrix $\boldsymbol{\epsilon}_0$ we could prescribe the special Dirichlet boundary conditions

$$\mathbf{u}(\mathbf{x}) = \boldsymbol{\epsilon}_0\mathbf{x}, \quad \text{for } \mathbf{x} \in \partial\Omega, \tag{8.5}$$

and measure $\boldsymbol{\tau}_0 = \langle \boldsymbol{\tau} \rangle$. Here, according to (8.4), $\boldsymbol{\epsilon}_0$ equals $\langle \boldsymbol{\epsilon} \rangle$. Since $\boldsymbol{\tau}_0$ is linearly related to $\boldsymbol{\epsilon}_0$ we can write

$$\boldsymbol{\tau}_0 = \boldsymbol{\mathcal{C}}^D\boldsymbol{\epsilon}_0, \tag{8.6}$$

which defines the elasticity tensor $\boldsymbol{\sigma}^D$ (D for Dirichlet). Alternatively for any symmetric matrix $\boldsymbol{\tau}_0$ we could prescribe the special Neumann boundary conditions

$$\boldsymbol{\tau}(\mathbf{x}) \cdot \mathbf{n} = \boldsymbol{\tau}_0 \cdot \mathbf{n}, \quad \text{for } \mathbf{x} \in \partial\Omega, \tag{8.7}$$

and measure $\boldsymbol{\epsilon}_0 = \langle \boldsymbol{\epsilon} \rangle$. Here, according to (8.4), $\boldsymbol{\tau}_0$ equals $\langle \boldsymbol{\tau} \rangle$. Since $\boldsymbol{\epsilon}_0$ is linearly related to $\boldsymbol{\tau}_0$ we can write

$$\boldsymbol{\epsilon}_0 = (\boldsymbol{\mathcal{C}}^N)^{-1}\boldsymbol{\tau}_0, \tag{8.8}$$

which defines the elasticity tensor $\boldsymbol{\sigma}^N$ (D for Dirichlet). It is easy to check that $\boldsymbol{\mathcal{C}}^D$ and $\boldsymbol{\mathcal{C}}^N$ satisfy all the usual symmetries of elasticity tensors.

Directly analogous to (3.13) we have the bounds

$$\langle \boldsymbol{\mathcal{C}}^{-1} \rangle^{-1} \leq \boldsymbol{\mathcal{C}}^D \leq \langle \boldsymbol{\mathcal{C}} \rangle, \qquad \langle \boldsymbol{\mathcal{C}}^{-1} \rangle^{-1} \leq \boldsymbol{\mathcal{C}}^N \leq \langle \boldsymbol{\mathcal{C}} \rangle \tag{8.9}$$

19

of (Nemat-Nasser and Hori 1993), and directly analogous to (3.14) for any boundary condition (not just the special boundary conditions (8.5) and (8.7)) we have the bounds

$$\langle \boldsymbol{\epsilon} \cdot \boldsymbol{\tau} \rangle \geq \boldsymbol{\epsilon}_0 \cdot \boldsymbol{\sigma}^N \boldsymbol{\epsilon}_0, \quad \langle \boldsymbol{\epsilon} \cdot \boldsymbol{\tau} \rangle \geq \boldsymbol{\tau}_0 (\boldsymbol{\sigma}^D)^{-1} \boldsymbol{\tau}_0, \tag{8.10}$$

where $\boldsymbol{\epsilon}_0 = \langle \boldsymbol{\epsilon} \rangle$ and $\boldsymbol{\tau}_0 = \langle \boldsymbol{\tau} \rangle$, due to Willis in 1989 private communication to Nemat-Nasser and Hori and presented by Nemat-Nasser and Hori (1993).

Also directly analogous to (5.9) and (5.20) we have the bounds

$$\boldsymbol{\mathcal{C}}^N \leq \boldsymbol{\mathcal{C}}^* \leq \boldsymbol{\mathcal{C}}^D, \tag{8.11}$$

where $\boldsymbol{\mathcal{C}}^*$ is the effective elasticity tensor of any assemblage of rescaled copies of Ω packed to fill all space. These are essentially the bounds of Huet (1990) applied to this assemblage. Thus "lower bounds" on $\boldsymbol{\mathcal{C}}^*$ directly give "lower bounds" on $\boldsymbol{\mathcal{C}}^D$ and "upper bounds" on $\boldsymbol{\mathcal{C}}^*$ directly give "upper bounds" on $\boldsymbol{\mathcal{C}}^N$. In particular, in two dimensions lower and upper bounds on $\boldsymbol{\epsilon}_0 \cdot \boldsymbol{\mathcal{C}}^* \boldsymbol{\epsilon}_0$ have been obtained by Gibiansky and Cherkaev (1984) (for the equivalent plate equation) and also by Allaire and Kohn (1993a). Assuming that the phases have been labeled so that $\mu_1 \geq \mu_2$ ($\kappa_1 - \kappa_2$ could be either positive or negative) and letting ϵ_1 and ϵ_2 denote the two eigenvalues $\boldsymbol{\epsilon}_0$, the bounds imply

$$\boldsymbol{\epsilon}_0 \cdot \boldsymbol{\mathcal{C}}^D \boldsymbol{\epsilon}_0 \geq (\epsilon_1 + \epsilon_2)^2 / (f_1/\kappa_1 + f_2/\kappa_2) + (\epsilon_1 - \epsilon_2)^2 / (f_1/\mu_1 + f_2/\mu_2),$$
$$\text{if} \quad |\kappa_1 - \kappa_2|(f_1\mu_2 + f_2\mu_1)|\epsilon_1 + \epsilon_2| \leq |\mu_1 - \mu_2|(f_1\kappa_2 + f_2\kappa_1)|\epsilon_1 - \epsilon_2|;$$

$$\boldsymbol{\epsilon}_0 \cdot \boldsymbol{\mathcal{C}}^D \boldsymbol{\epsilon}_0 \geq (\epsilon_1 + \epsilon_2)^2 (f_1\kappa_1 + f_2\kappa_2) + (\epsilon_1 - \epsilon_2)^2 (f_1\mu_1 + f_2\mu_2)$$
$$- f_1 f_2 \frac{[|\kappa_1 - \kappa_2||\epsilon_1 + \epsilon_2| + |\mu_1 - \mu_2||\epsilon_1 - \epsilon_2|]^2}{f_1(\mu_2 + \kappa_2) + f_2(\mu_1 + \kappa_1)},$$
$$\text{if} \quad (\mu_2 + f_1\kappa_2 + f_2\kappa_1)|\epsilon_1 - \epsilon_2| \geq f_2|\kappa_1 - \kappa_2||\epsilon_1 + \epsilon_2|$$
$$\text{and} \quad |\kappa_1 - \kappa_2|(f_1\mu_2 + f_2\mu_1)|\epsilon_1 + \epsilon_2| \geq |\mu_1 - \mu_2|(f_1\kappa_2 + f_2\kappa_1)|\epsilon_1 - \epsilon_2|;$$

$$\boldsymbol{\epsilon}_0 \cdot \boldsymbol{\mathcal{C}}^D \boldsymbol{\epsilon}_0 \geq \mu_2(\epsilon_1 - \epsilon_2)^2 + \frac{\kappa_1\kappa_2 + \mu_2(f_1\kappa_1 + f_2\kappa_2)}{\mu_2 + f_1\kappa_2 + f_2\kappa_1}(\epsilon_1 + \epsilon_2)^2,$$
$$\text{if} \quad (\mu_2 + f_1\kappa_2 + f_2\kappa_1)|\epsilon_1 - \epsilon_2| \leq f_2|\kappa_1 - \kappa_2||\epsilon_1 + \epsilon_2|; \tag{8.12}$$

and

$$\boldsymbol{\epsilon}_0 \cdot \boldsymbol{\mathcal{C}}^N \boldsymbol{\epsilon}_0 \leq (\epsilon_1 + \epsilon_2)^2 (f_1\kappa_1 + f_2\kappa_2) + (\epsilon_1 - \epsilon_2)^2 (f_1\mu_1 + f_2\mu_2)$$
$$- f_1 f_2 \frac{[|\kappa_1 - \kappa_2||\epsilon_1 + \epsilon_2| - |\mu_1 - \mu_2||\epsilon_1 - \epsilon_2|]^2}{f_1(\mu_2 + \kappa_2) + f_2(\mu_1 + \kappa_1)},$$
$$\text{if} \quad f_1|\kappa_1 - \kappa_2||\epsilon_1 + \epsilon_2| \leq (\mu_1 + f_1\kappa_2 + f_2\kappa_1)|\epsilon_1 - \epsilon_2|$$
$$\text{and} \quad f_+|\mu_1 - \mu_2||\epsilon_1 - \epsilon_2| \leq (\kappa_+ + f_1\mu_2 + f_2\mu_1)|\epsilon_1 + \epsilon_2|;$$

$$\boldsymbol{\epsilon}_0 \cdot \boldsymbol{\mathcal{C}}^N \boldsymbol{\epsilon}_0 \leq \mu_1(\epsilon_1 - \epsilon_2)^2 + \frac{\kappa_1\kappa_2 + \mu_1(f_1\kappa_1 + f_2\kappa_2)}{\mu_1 + f_1\kappa_2 + f_2\kappa_1}(\epsilon_1 + \epsilon_2)^2,$$
$$\text{if} \quad f_1|\kappa_1 - \kappa_2||\epsilon_1 + \epsilon_2| \geq (\mu_1 + f_1\kappa_2 + f_2\kappa_1)|\epsilon_1 - \epsilon_2|;$$

$$\boldsymbol{\epsilon}_0 \cdot \boldsymbol{\mathcal{C}}^N \boldsymbol{\epsilon}_0 \leq \kappa_+(\epsilon_1 + \epsilon_2)^2 + \frac{\mu_1\mu_2 + \kappa_+(f_1\mu_1 + f_2\mu_2)}{\kappa_+ + f_1\mu_2 + f_2\mu_1}(\epsilon_1 - \epsilon_2)^2,$$
$$\text{if} \quad f_+|\mu_1 - \mu_2||\epsilon_1 - \epsilon_2| \geq (\kappa_+ + f_1\mu_2 + f_2\mu_1)|\epsilon_1 + \epsilon_2|, \tag{8.13}$$

20

where κ_+ is the maximum of κ_1 and κ_2 and f_+ is the volume fraction of the material corresponding to κ_+.

The corresponding three-dimensional bounds follow directly from (8.11) and the bounds of Allaire and Kohn (1993b), but are not so explicit. Assuming that the Lame moduli

$$\lambda_1 = \kappa_1 - 2\mu_1/3 \ \text{ and } \ \lambda_2 = \kappa_2 - 2\mu_2/3 \tag{8.14}$$

of both phases are positive, and that the bulk and shear moduli of the two phases are well-ordered with

$$\kappa_1 > \kappa_2 > 0 \ \text{ and } \ \mu_1 > \mu_2 > 0, \tag{8.15}$$

these bounds are

$$\boldsymbol{\epsilon}_0 : \boldsymbol{\mathcal{C}}^D \boldsymbol{\epsilon}_0 \geq \boldsymbol{\epsilon}_0 : \boldsymbol{\mathcal{C}}_2 \boldsymbol{\epsilon}_0 + f_1 \max_{\boldsymbol{\eta}} [2 \boldsymbol{\epsilon}_0 : \boldsymbol{\eta} - \boldsymbol{\eta} : (\boldsymbol{\mathcal{C}}_1 - \boldsymbol{\mathcal{C}}_2)^{-1} \boldsymbol{\eta} - f_2 g(\boldsymbol{\eta})],$$

$$\boldsymbol{\epsilon}_0 : \boldsymbol{\mathcal{C}}^N \boldsymbol{\epsilon}_0 \geq \boldsymbol{\epsilon}_0 : \boldsymbol{\mathcal{C}}_1 \boldsymbol{\epsilon}_0 + f_2 \min_{\boldsymbol{\eta}} [2 \boldsymbol{\epsilon}_0 : \boldsymbol{\eta} + \boldsymbol{\eta} : (\boldsymbol{\mathcal{C}}_1 - \boldsymbol{\mathcal{C}}_2)^{-1} \boldsymbol{\eta} - f_1 h(\boldsymbol{\eta})], \tag{8.16}$$

where $g(\boldsymbol{\eta})$ and $h(\boldsymbol{\eta})$ are function of the eigenvalues η_1, η_2, and η_3 of the symmetric matrix $\boldsymbol{\eta}$. Assuming that these are labeled with

$$\eta_1 \leq \eta_2 \leq \eta_3, \tag{8.17}$$

we have

$$g(\boldsymbol{\eta}) = \frac{(\eta_1 - \eta_3)^2}{4\mu_2} + \frac{(\eta_1 + \eta_3)^2}{4(\lambda_2 + \mu_2)} \ \text{ if } \ \eta_3 \geq \frac{\lambda_2 + 2\mu_2}{2(\lambda_2 + \mu_2)}(\eta_1 + \eta_3) \geq \eta_1,$$

$$g(\boldsymbol{\eta}) = \frac{\eta_1^2}{\lambda_2 + 2\mu_2} \ \text{ if } \ \eta_1 > \frac{\lambda_2 + 2\mu_2}{2(\lambda_2 + \mu_2)}(\eta_1 + \eta_3),$$

$$g(\boldsymbol{\eta}) = \frac{\eta_3^2}{\lambda_2 + 2\mu_2} \ \text{ if } \ \eta_3 < \frac{\lambda_2 + 2\mu_2}{2(\lambda_2 + \mu_2)}(\eta_1 + \eta_3), \tag{8.18}$$

and

$$h(\boldsymbol{\eta}) = \frac{1}{\lambda_1 + 2\mu_1} \min\{\eta_1^2, \eta_2^2, \eta_3^2\}. \tag{8.19}$$

The bounds (8.12), (8.13) and (8.16) can be used in an inverse way to bound the volume fraction $f_1 = 1 - f_2$, for a single experiment when for special Dirichlet conditions $\boldsymbol{\epsilon}_0$ is prescribed and $\boldsymbol{\tau}_0 \ (= \boldsymbol{\mathcal{C}}^D \boldsymbol{\epsilon}_0)$ is measured, or when for special Neumann conditions $\boldsymbol{\tau}_0$ is prescribed and $\boldsymbol{\epsilon}_0 \ (= \boldsymbol{\mathcal{C}}^N \boldsymbol{\epsilon}_0)$ is measured. Allaire and Kohn (1993b) also derive bounds on the complementary energy and these imply

$$\boldsymbol{\tau}_0 : (\boldsymbol{\mathcal{C}}^N)^{-1} \boldsymbol{\tau}_0 \geq \boldsymbol{\tau}_0 : \boldsymbol{\mathcal{C}}_1^{-1} \boldsymbol{\tau}_0 + f_2 \max_{\boldsymbol{\zeta}} [2 \boldsymbol{\tau}_0 : \boldsymbol{\zeta} - \boldsymbol{\zeta} : (\boldsymbol{\mathcal{C}}_2^{-1} - \boldsymbol{\mathcal{C}}_1^{-1})^{-1} \boldsymbol{\zeta} - f_1 \boldsymbol{\zeta} : \boldsymbol{\mathcal{C}}_1 \boldsymbol{\zeta} + f_1 h(\boldsymbol{\mathcal{C}}_1 \boldsymbol{\zeta})],$$

$$\tag{8.20}$$

and

$$\boldsymbol{\tau}_0 : (\boldsymbol{\mathcal{C}}^D)^{-1} \boldsymbol{\tau}_0 \leq \boldsymbol{\tau}_0 : \boldsymbol{\mathcal{C}}_2^{-1} \boldsymbol{\tau}_0 + f_1 \min_{\boldsymbol{\zeta}} [2 \boldsymbol{\tau}_0 : \boldsymbol{\zeta} + \boldsymbol{\zeta} : (\boldsymbol{\mathcal{C}}_2^{-1} - \boldsymbol{\mathcal{C}}_1^{-1})^{-1} \boldsymbol{\zeta} - f_2 \boldsymbol{\zeta} : \boldsymbol{\mathcal{C}}_2 \boldsymbol{\zeta} + f_2 g(\boldsymbol{\mathcal{C}}_2 \boldsymbol{\zeta})].$$

$$\tag{8.21}$$

The bound in (8.20) is particularly useful when $\boldsymbol{\tau}_0 = -p\mathbf{I}$, corresponding to immersing the body Ω in a fluid with pressure p. Then from measurements of the resulting volume

change of the body one can determine $\boldsymbol{\tau}_0 : (\boldsymbol{\mathcal{C}}^N)^{-1}\boldsymbol{\tau}_0 = -p\operatorname{Tr}\boldsymbol{\epsilon}_0$. Let us assume $\lambda_1 > 0$ and set $\boldsymbol{\zeta} = \alpha\mathbf{I} + \mathbf{A}$, with $\mathbf{A}$ being a trace free matrix with eigenvalues a_1, a_2 and a_3. Then we have $\boldsymbol{\eta} = \boldsymbol{\mathcal{C}}_1\boldsymbol{\zeta} = 2\mu_1(k\mathbf{I} + \mathbf{A})$ where $k = \alpha[1 + 3\lambda_1/(2\mu_1)]$. Substitution gives

$$
\begin{aligned}
&[\boldsymbol{\zeta} : \boldsymbol{\mathcal{C}}_1\boldsymbol{\zeta} - h(\boldsymbol{\mathcal{C}}_1\boldsymbol{\zeta})] - \alpha^2[\mathbf{I} : \boldsymbol{\mathcal{C}}_1\mathbf{I} - h(\boldsymbol{\mathcal{C}}_1\mathbf{I})] \\
&= 2\mu_1\left[a_1^2 + a_2^2 + a_3^2 - \frac{2\mu_1}{\lambda_1 + 2\mu_1}\min\{(k+a_1)^2 - k^2, (k+a_2)^2 - k^2, (k+a_3)^2 - k^2\}\right] \\
&\geq 2\mu_1[a_1^2 + a_2^2 + a_3^2 - \min\{2a_1k + a_1^2, 2a_2k + a_2^2, 2a_3k + a_3^2\}],
\end{aligned}
\tag{8.22}
$$

which is surely positive since $\min\{2a_1k + a_1^2, 2a_2k + a_2^2, 2a_3k + a_3^2\} \leq a_j^2$ where j is such that ka_j is non-positive. (Note that a_1, a_2 and a_3 cannot all have the same sign since they sum to zero). Consequently when $\boldsymbol{\tau}_0 = -p\mathbf{I}$ the maximum over $\boldsymbol{\zeta}$ in (8.20) is achieved when $\mathbf{A} = 0$ and taking the maximum over α gives

$$
-p\operatorname{Tr}\boldsymbol{\epsilon}_0 \geq p^2\left[\frac{1}{\kappa_1} + \frac{f_2}{\frac{\kappa_1\kappa_2}{\kappa_1 - \kappa_2} + \frac{4f_1\mu_1\kappa_1}{3\kappa_1 + 4\mu_1}}\right],
\tag{8.23}
$$

or equivalently

$$
-p/(\operatorname{Tr}\boldsymbol{\epsilon}_0) \leq \kappa_{HSH}^+ \equiv \kappa_1 - \frac{f_2}{1/(\kappa_1 - \kappa_2) - f_1/(\kappa_1 + 4\mu_1/3)},
\tag{8.24}
$$

where κ_{HSH}^+ is the upper bulk modulus bound of Hashin and Shtrikman (1963) and Hill (1963). The inequality (8.23) can be rewritten as

$$
\frac{f_2}{-(\operatorname{Tr}\boldsymbol{\epsilon}_0/p) - 1/\kappa_1} \leq \frac{\kappa_1\kappa_2}{\kappa_1 - \kappa_2} + \frac{4f_1\mu_1\kappa_1}{3\kappa_1 + 4\mu_1},
\tag{8.25}
$$

where we have used the fact that $-(\operatorname{Tr}\boldsymbol{\epsilon}_0/p) - 1/\kappa_1$ is positive (since $\boldsymbol{\tau}_0 : (\boldsymbol{\mathcal{C}}^N)^{-1}\boldsymbol{\tau}_0 \geq \boldsymbol{\tau}_0 : (\boldsymbol{\mathcal{C}}_1)^{-1}\boldsymbol{\tau}_0$ by (8.9)). This then yields the volume fraction bound

$$
f_2 \leq \frac{\frac{\kappa_1\kappa_2}{\kappa_1 - \kappa_2} + \frac{4\mu_1\kappa_1}{3\kappa_1 + 4\mu_1}}{\frac{1}{-(\operatorname{Tr}\boldsymbol{\epsilon}_0/p) - 1/\kappa_1} + \frac{4\mu_1\kappa_1}{3\kappa_1 + 4\mu_1}},
\tag{8.26}
$$

which we expect to be closest to the actual volume fraction when phase 2 (the softer phase) is the inclusion phase. Thus the bound may be particularly effective for estimating the volume of cavities in a body. Note that if some granules of phase 1 lie within these cavities, then such granules will not contribute to this volume fraction estimate, but will contribute to the overall weight. If the weight of the body has been measured (and the density of phase 1 is known) this provides a way of estimating the volume of granules of phase 1 which lie within the cavities.

When multiple experiments have been done, and the full tensor $\boldsymbol{\mathcal{C}}^D$ or $\boldsymbol{\mathcal{C}}^N$ has been determined, then the "trace bounds" of Zhikov(1988, 1991) and Milton and Kohn (1988) can be used. (These generalize the well known Hashin-Shtrikman (1963) bounds to anisotropic elastic composites.) Define the two traces

$$
\operatorname{Tr}_h \boldsymbol{\mathcal{A}} = A_{iijj}/d, \qquad Tr_s\boldsymbol{\mathcal{A}} = A_{ijij} - (A_{iijj}/d),
\tag{8.27}
$$

for any fourth order tensor $\boldsymbol{\mathcal{A}}$ with elements $A_{ijk\ell}$ in spatial dimension d. Then, assuming the moduli of the two-phases are well ordered satisfying (8.15), their lower and upper "bulk modulus type bounds" imply, through (8.11), the universal bounds

$$f_1 \operatorname{Tr}_h[(\boldsymbol{\mathcal{C}}^D - \boldsymbol{\mathcal{C}}_2)^{-1}] \leq \frac{1}{d(\kappa_1 - \kappa_2)} + \frac{f_2}{d\kappa_2 + 2(d-1)\mu_2},$$

$$f_2 \operatorname{Tr}_h[(\boldsymbol{\mathcal{C}}_1 - \boldsymbol{\mathcal{C}}^N)^{-1}] \leq \frac{1}{d(\kappa_1 - \kappa_2)} - \frac{f_1}{d\kappa_1 + 2(d-1)\mu_1}, \qquad (8.28)$$

while their lower and upper "shear modulus type bounds," imply the universal bounds

$$f_1 \operatorname{Tr}_s[(\boldsymbol{\mathcal{C}}^D - \boldsymbol{\mathcal{C}}_2)^{-1}] \leq \frac{(d-1)(d+2)}{4(\mu_1 - \mu_2)} + \frac{d(d-1)(\kappa_2 + 2\mu_2)f_2}{2\mu_2(d\kappa_2 + 2(d-1)\mu_2)},$$

$$f_2 \operatorname{Tr}_s[(\boldsymbol{\mathcal{C}}_1 - \boldsymbol{\mathcal{C}}^N)^{-1}] \leq \frac{(d-1)(d+2)}{4(\mu_1 - \mu_2)} - \frac{d(d-1)(\kappa_1 + 2\mu_1)f_1}{2\mu_1(d\kappa_1 + 2(d-1)\mu_1)}. \qquad (8.29)$$

Since these inequalities depend linearly on $f_1 = 1 - f_2$ they can easily be inverted to obtain bounds on f_1 given $\boldsymbol{\mathcal{C}}^D$ or $\boldsymbol{\mathcal{C}}^N$.

As noted by Milton and Kohn (1988) the lower and upper "bulk modulus type bounds" are tighter than those obtained by Kantor and Bergman (1984) and Francfort and Murat (1986), which imply

$$\operatorname{Tr}_h \boldsymbol{\mathcal{C}}^N \leq d\kappa_1 - \frac{f_2}{\frac{1}{d(\kappa_1 - \kappa_2)} - \frac{f_1}{d\kappa_1 + 2(d-1)\mu_1}},$$

$$1/\operatorname{Tr}_h[(\boldsymbol{\mathcal{C}}^D)^{-1}] \geq d\kappa_2 + \frac{f_1}{\frac{1}{d(\kappa_1 - \kappa_2)} + \frac{f_2}{d\kappa_2 + 2(d-1)\mu_2}}. \qquad (8.30)$$

For bodies Ω of ellipsoidal or parallelopipedic shape the universal bounds (8.30) were obtained by Nemat-Nasser and Hori (1993, 1995): see the equations (4.3.9) and (4.4.8), with $I = 1$, in their 1995 paper. Their other bounds, with $I = 2$, which incorporate the "shear responses" of the tensors $\boldsymbol{\mathcal{C}}^N$ and $\boldsymbol{\mathcal{C}}^D$ are improved upon by the bounds (8.29) as can be seen using the inequality

$$\operatorname{Tr}_s \boldsymbol{\mathcal{A}}^{-1} \geq (d-1)^2 (d+2)^2 / (4 \operatorname{Tr}_s \boldsymbol{\mathcal{A}}), \qquad (8.31)$$

which holds for any positive definite fourth-order tensor $\boldsymbol{\mathcal{A}}$.

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U(σ₁)/f₁ → $U(\sigma_1)/f_1$

L(σ₁)/f₁ → $L(\sigma_1)/f_1$

σ_1